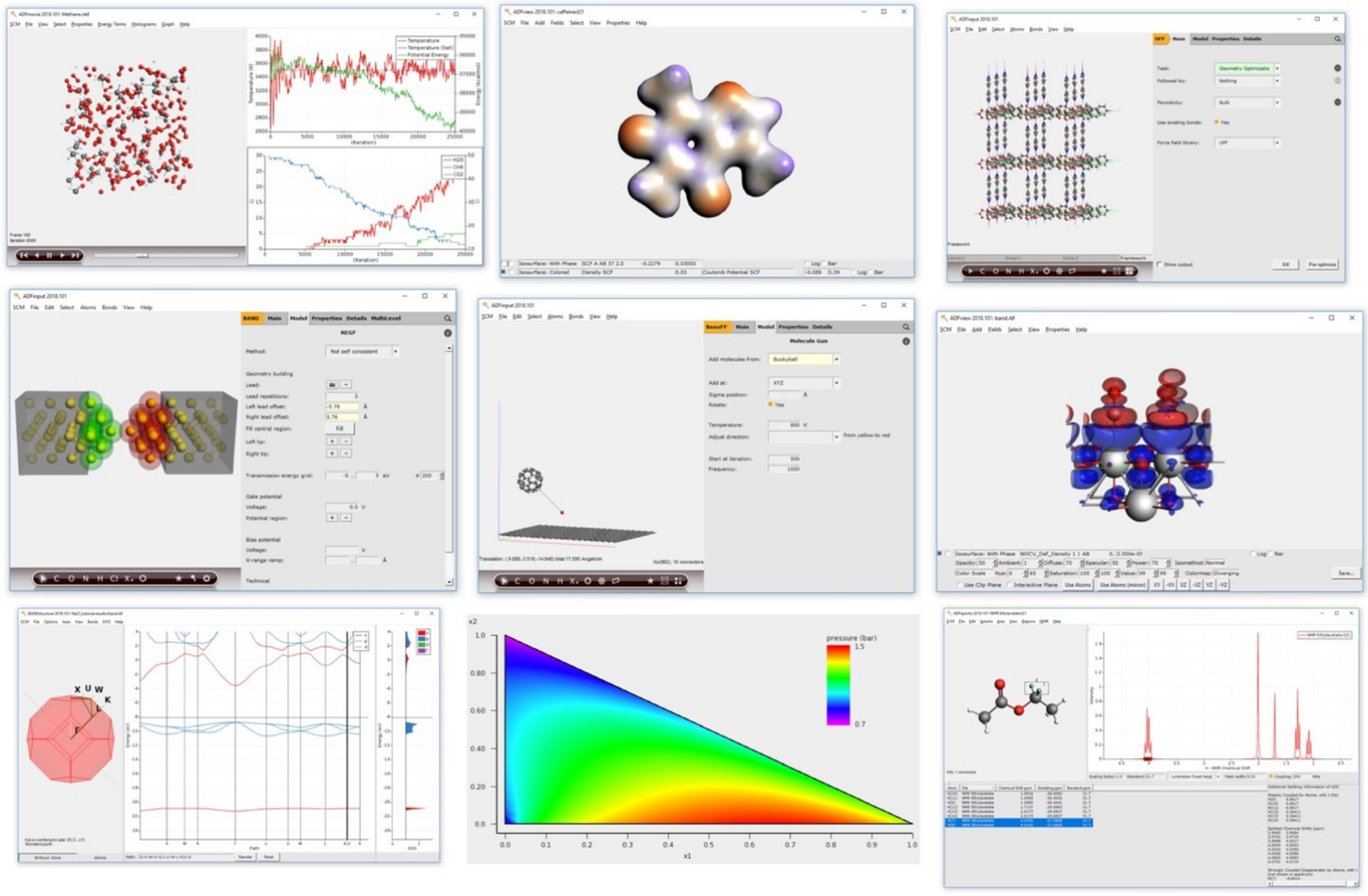
Online workshop:
Chemistry & Materials
with the Amsterdam Modeling Suite



Virtual Winter School on Computational Chemistry, 20 February 2020

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SCM
Software for
Chemistry &
Materials

Program

- 10.30-13.00: hands-on 1: molecules
  - Short introduction Amsterdam Modeling Suite & its Graphical Interface
  - Building & importing molecules and structures
  - Calculating spectroscopy properties: IR, UV/VIS, NMR
  - Conformers & Potential Energy Surfaces
  - Transition States

- 14.00-15.00: general Q&A + discussion

- 15.00-15.30: virtual coffee break

- 15.30-18.00: hands-on 2: periodic systems
  - Importing cif files, structure database, slicing surfaces, polymers and nanotubes
  - Electronic structure and properties of semiconductors
  - Mechanical properties of polymers
  - Molecule gun for high-impact processes and deposition
  - Battery discharge with Grand Canonical Monte Carlo

Background: SCM, ADF & AMS

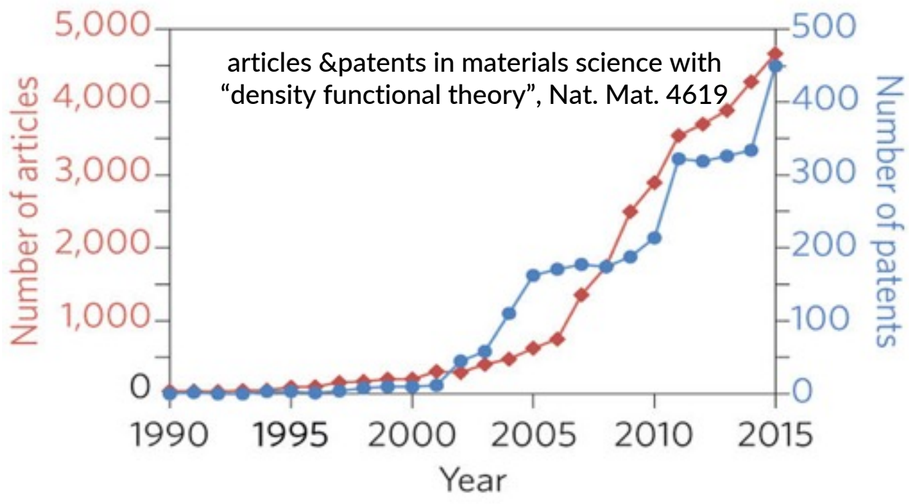
- ADF = first DFT code for chemistry (1970s)
  Baerends@VU (>'73), Ziegler@Calgary(+) (>'75)
  - 80s: support industrial users Mitsui, Shell, Akzo, Unilever

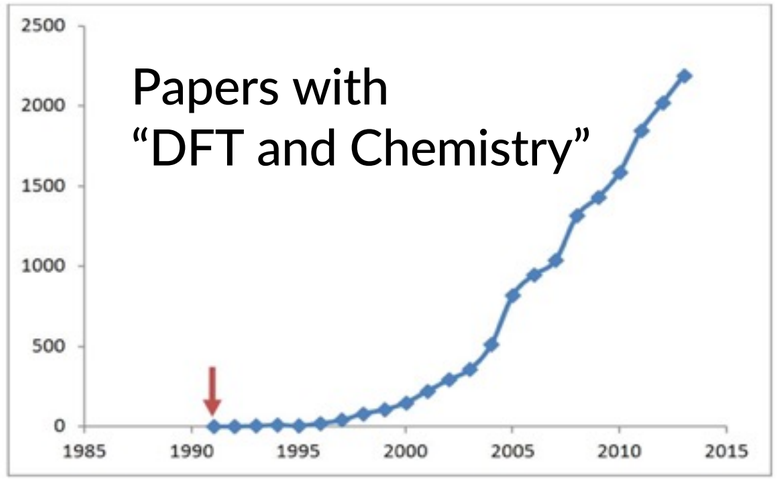
- SCM: Spin-off company 1995

- 21 people (15 senior PhD's) + 3 EU fellows

- Many academic collaborators / EU networks
  - ~150 authors
  - New functionality
  - Academia, government & industry users worldwide

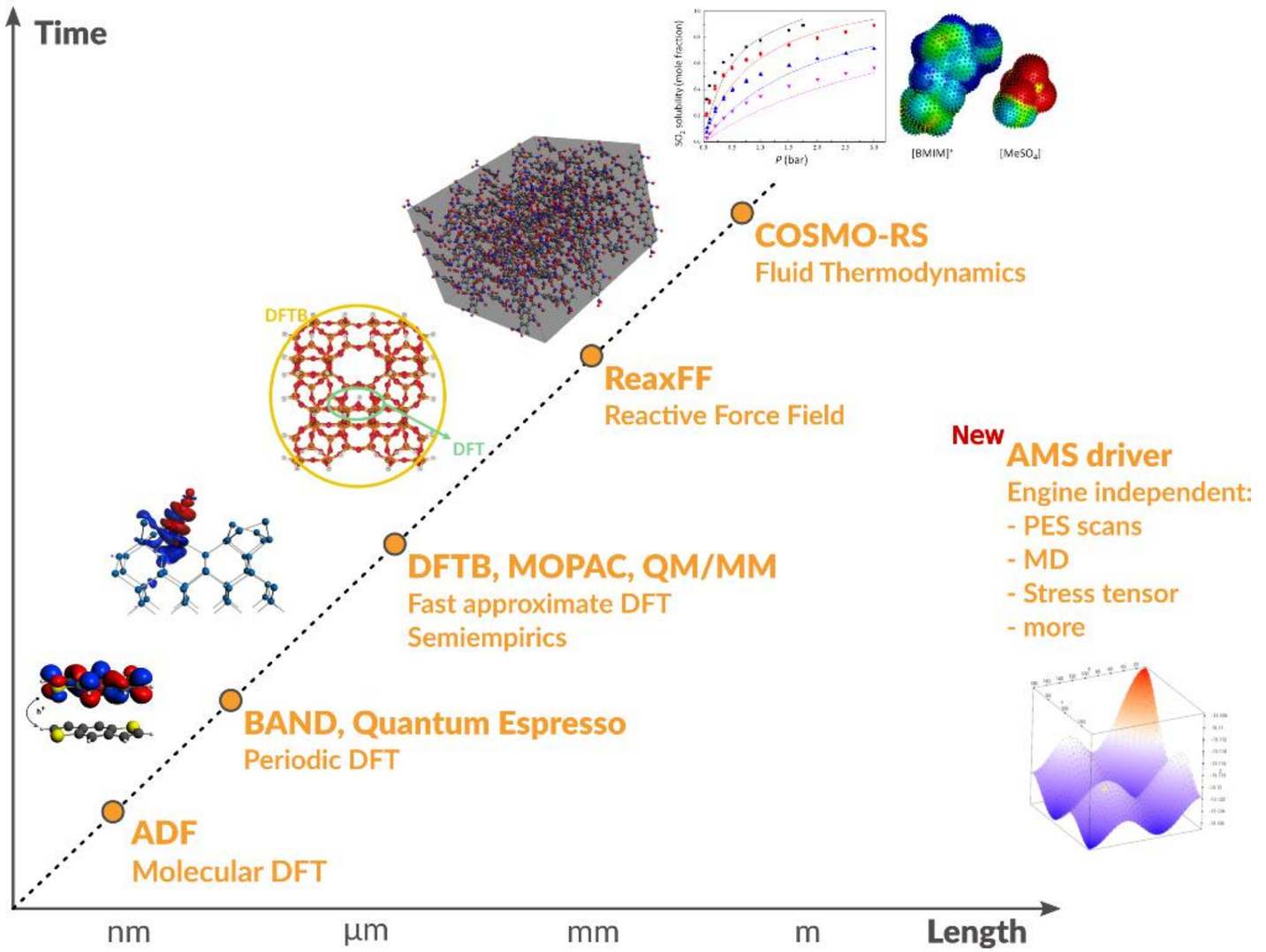
- SCM: development, debug,
port, optimize, docs & <u>support</u>



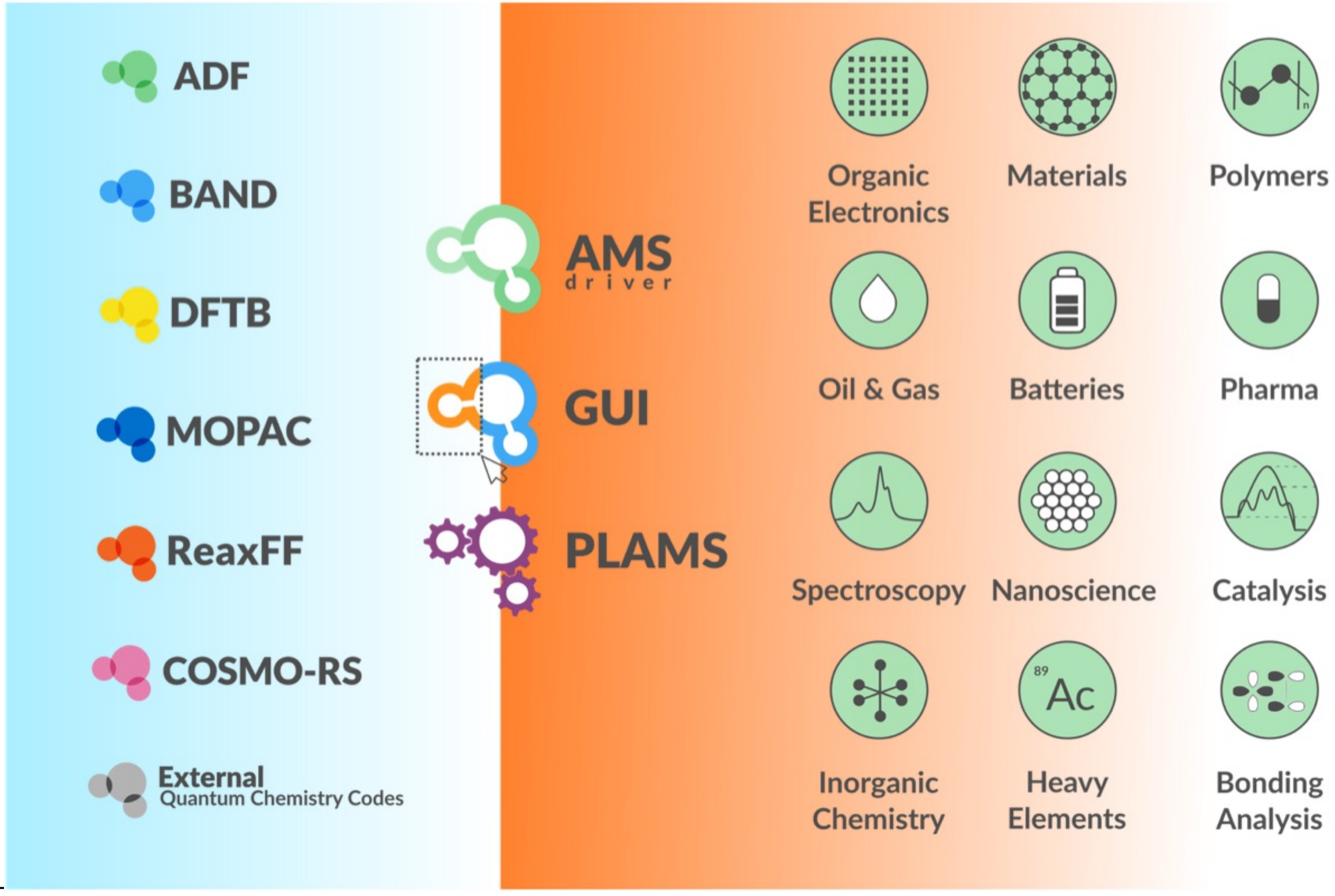


Amsterdam Modeling Suite

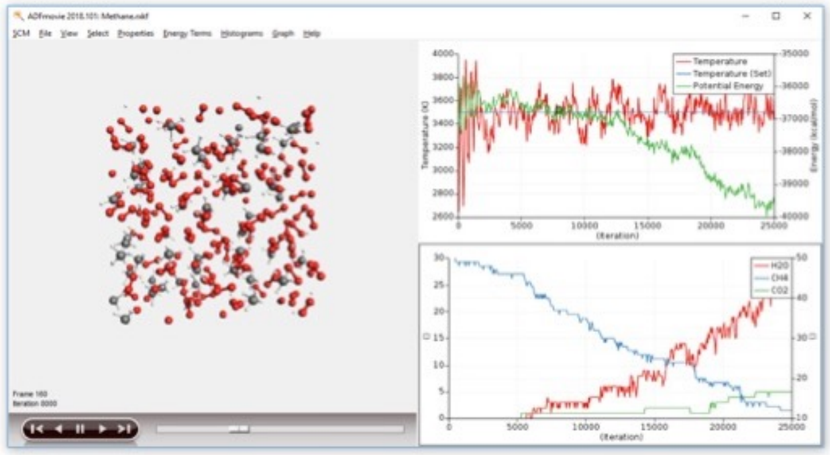
- ADF: powerful molecular DFT
  - Spectroscopy: NMR, EPR, VCD, UV, XAS
  - Advanced solvation / environments
- BAND: periodic DFT
  - (2D) Materials, spectroscopy, analysis
- Interface with and binaries for QE
- DFTB & MOPAC
  fast electronic structure
- ReaxFF: Reactive MD
  - Dynamics of large complicated systems
- COSMO-RS: fluid thermodynamics
  - VLE, LLE, logP, solubility
- Integrated GUI: use out of the box
- Scripting: workflows & automation

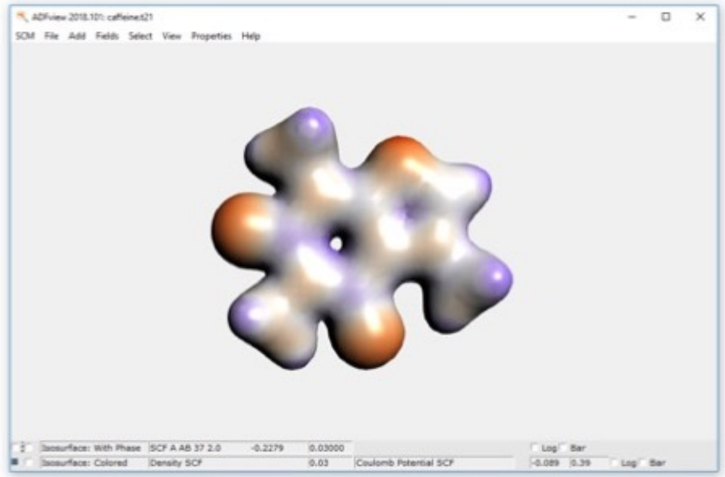


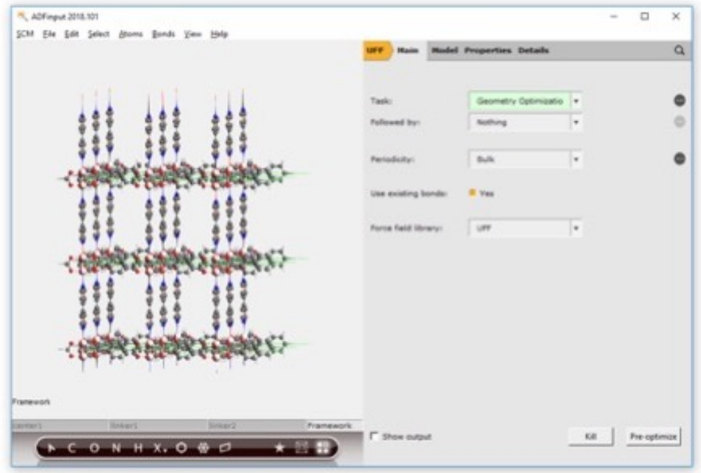
AMSdriver, PLAMS & GUI

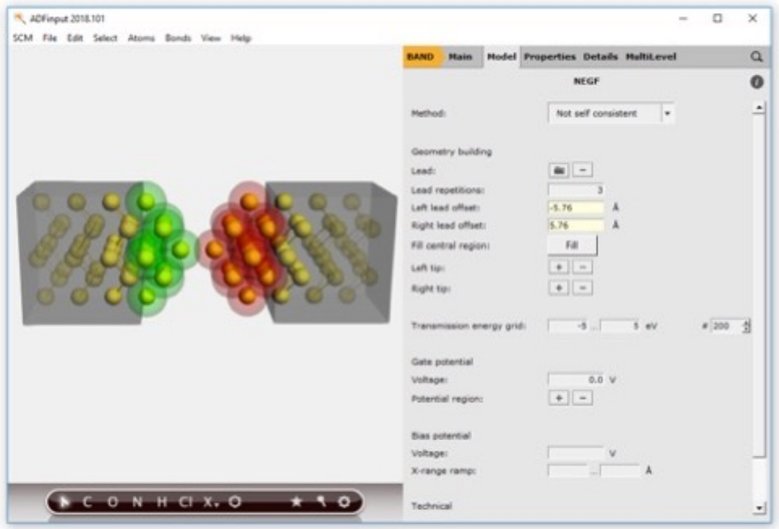


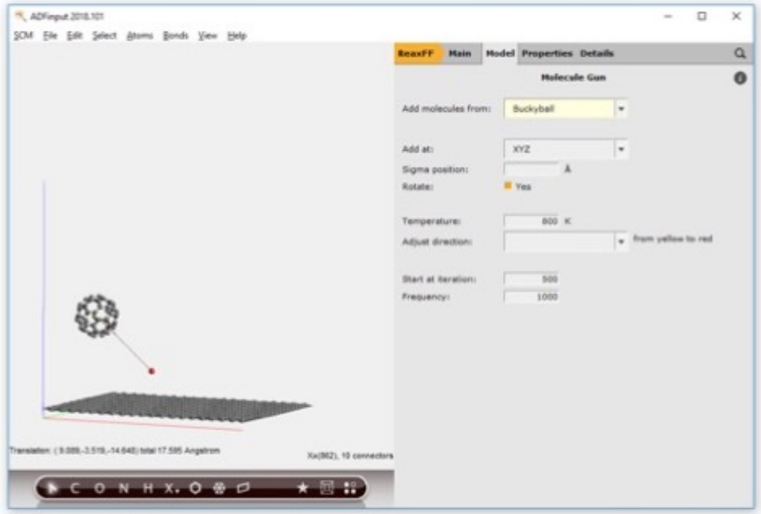
1 GUI: build, run & analyze

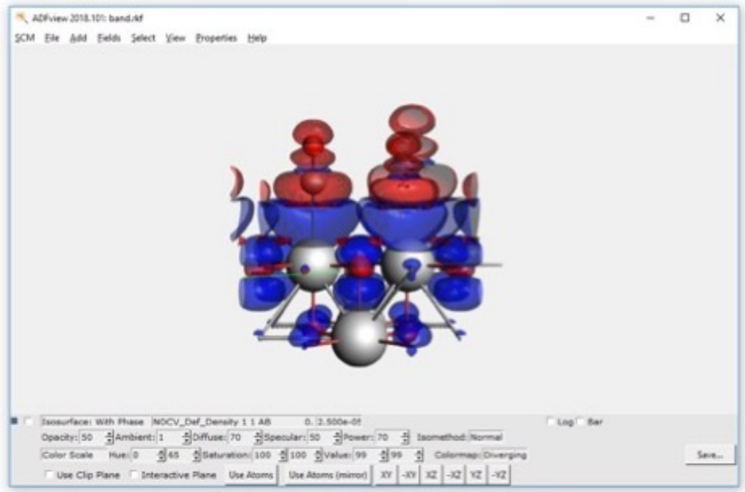


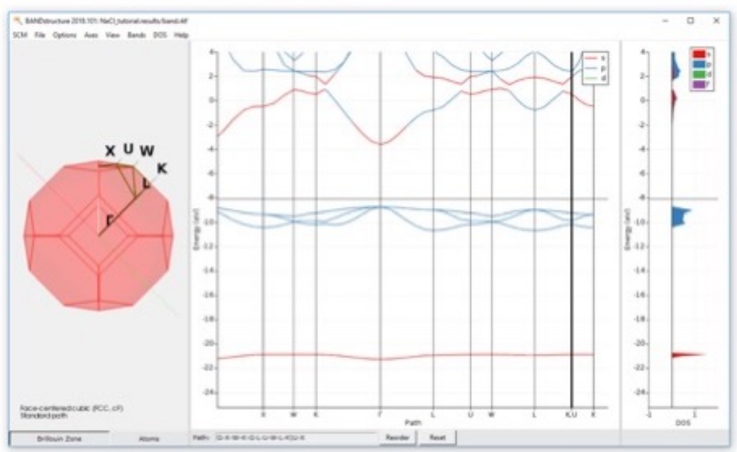


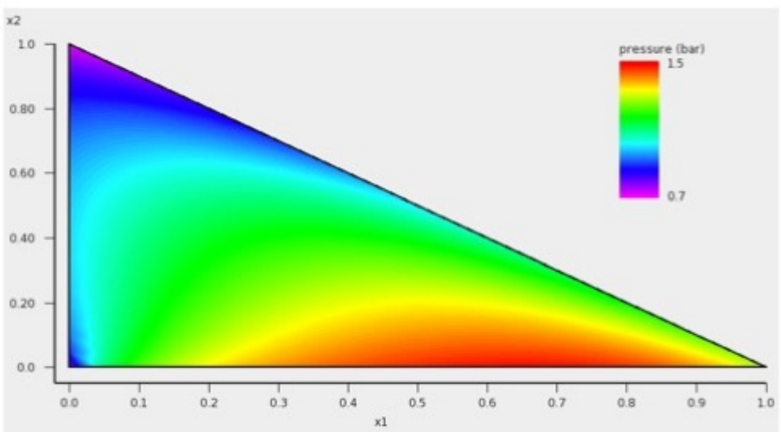


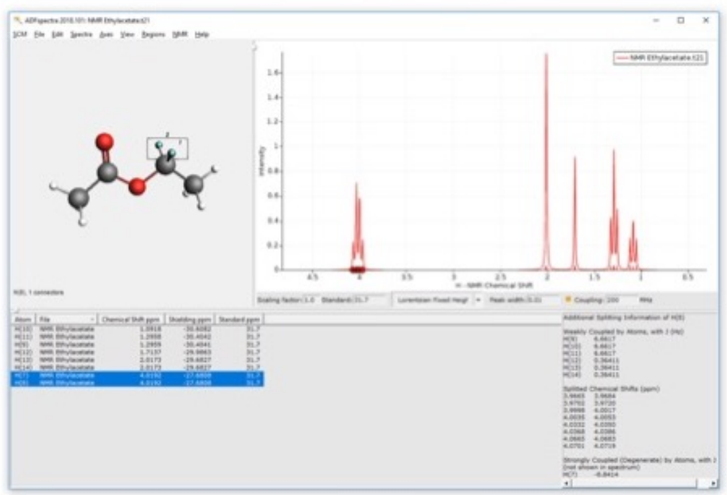






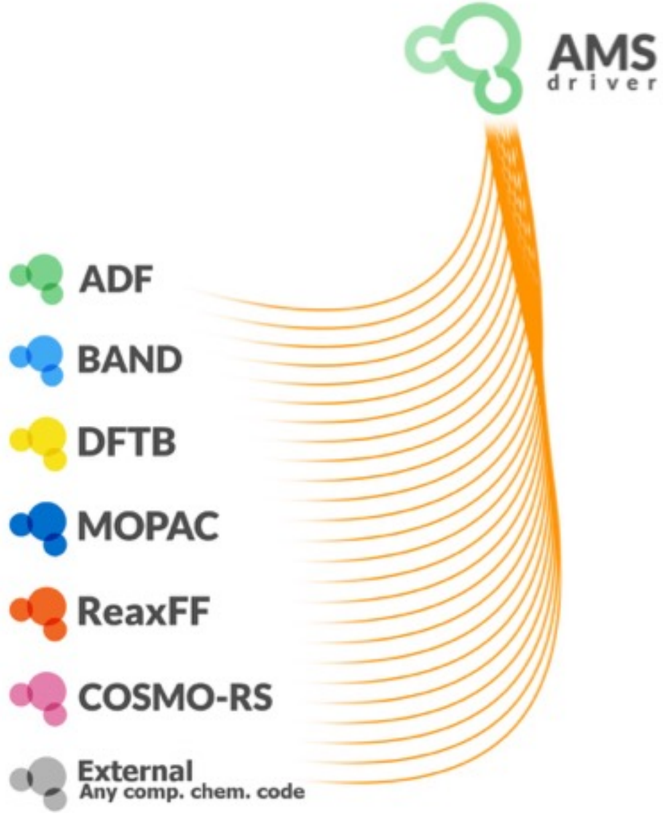


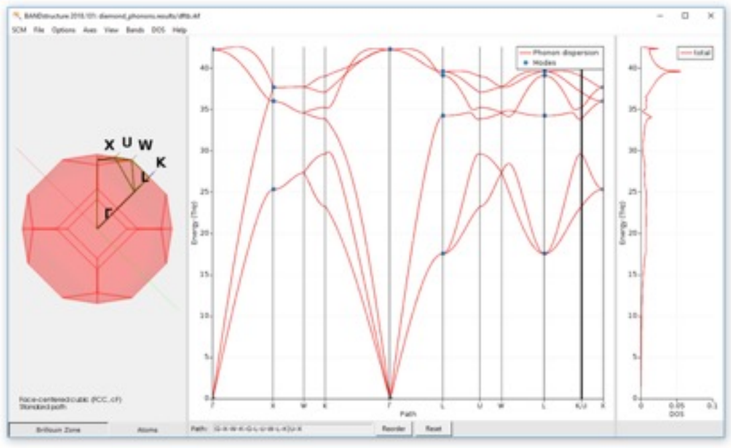


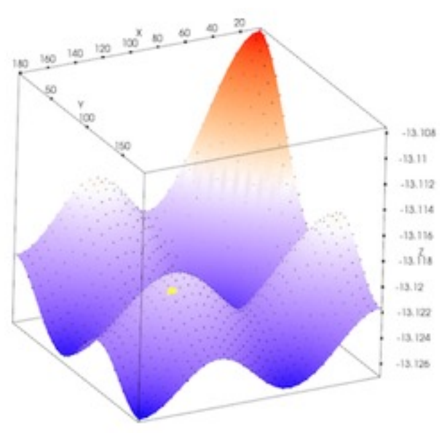


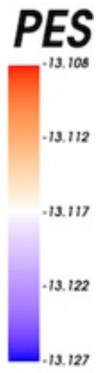
The AMS driver: decouple from Engine

- Frequencies (+ analysis) & phonons
- Stress & elastic tensors
- Scan (multiple) coords, any periodicity
- Geometries, TS, IRC
- Advanced Molecular Dynamics
- (Grand Canonical) Monte Carlo

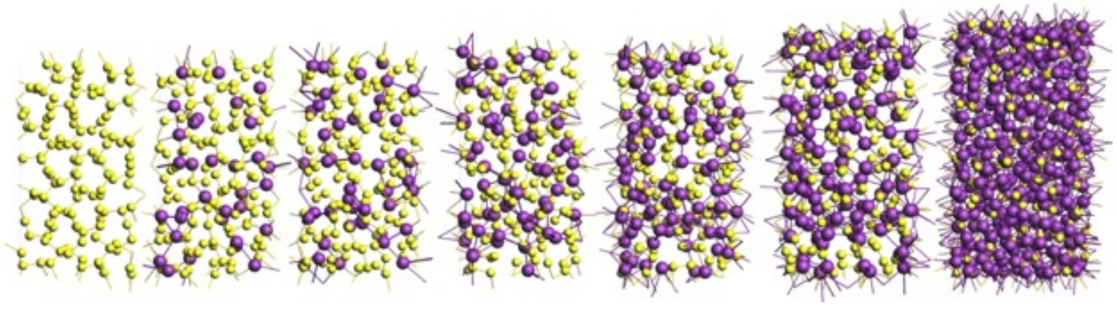




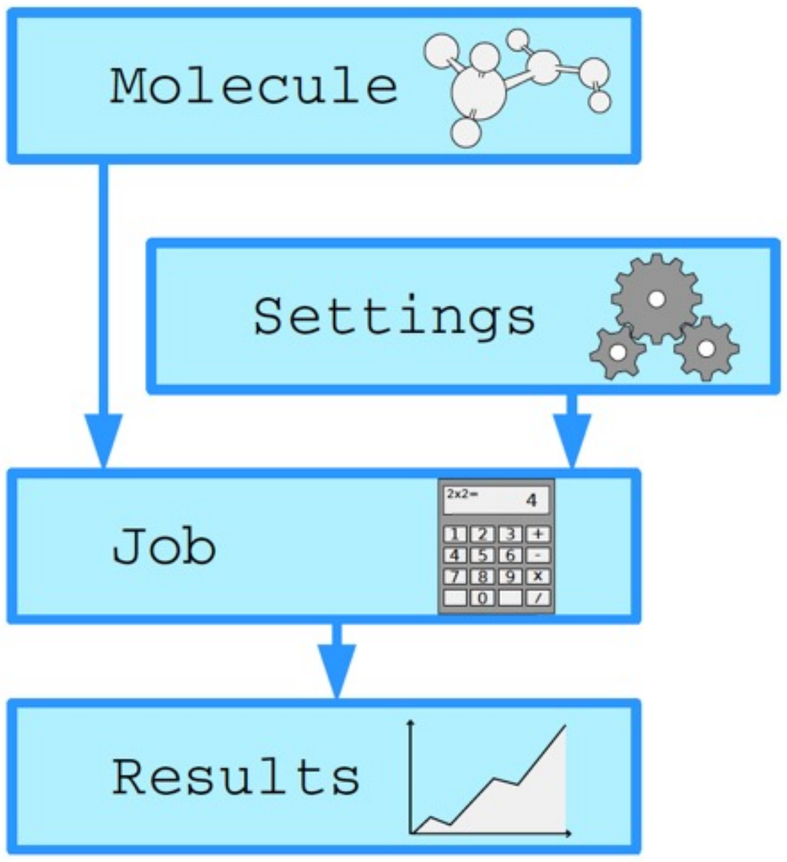


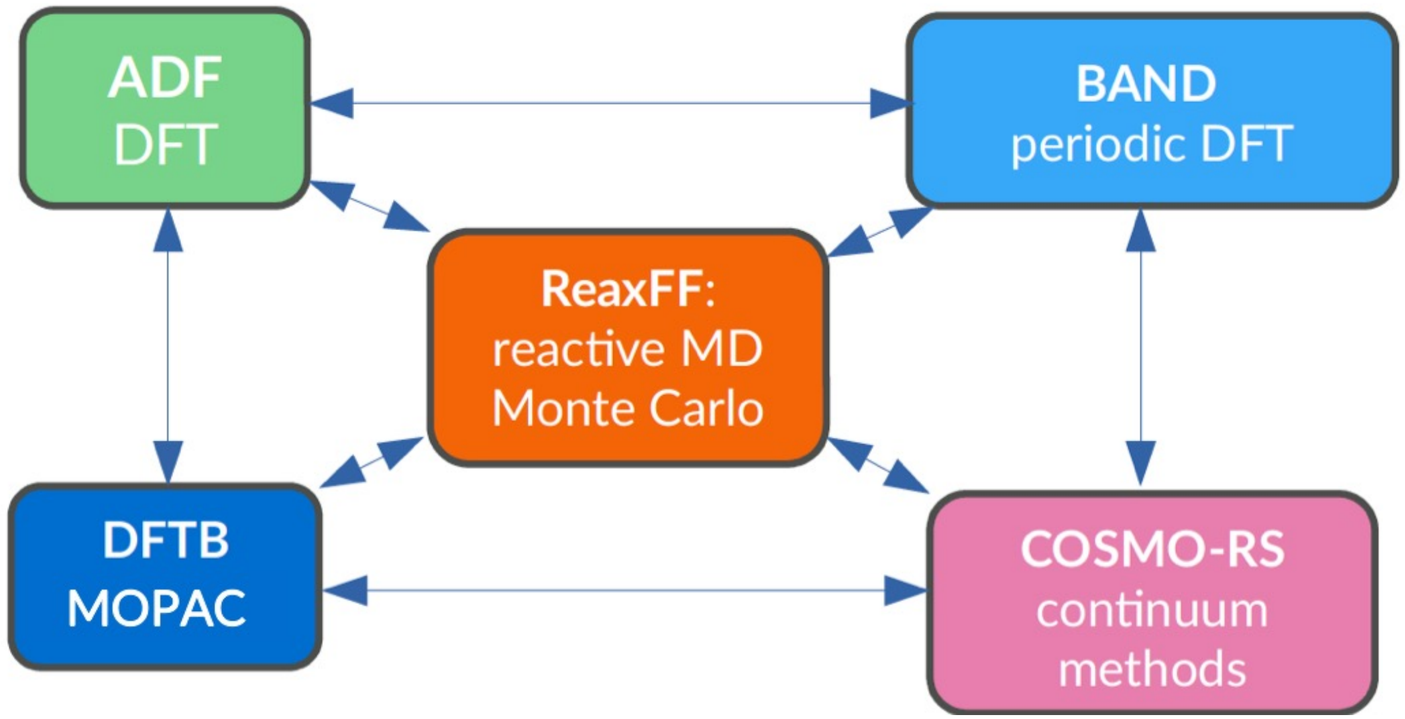


$S_8 \longrightarrow Li_2S_8 \longrightarrow Li_2S_6 \longrightarrow Li_2S_4 \longrightarrow Li_2S_3 \longrightarrow Li_2S_2 \longrightarrow Li_2S$



PLAMS: python scripting



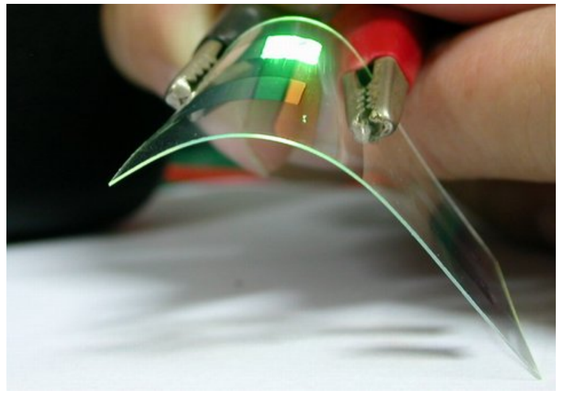


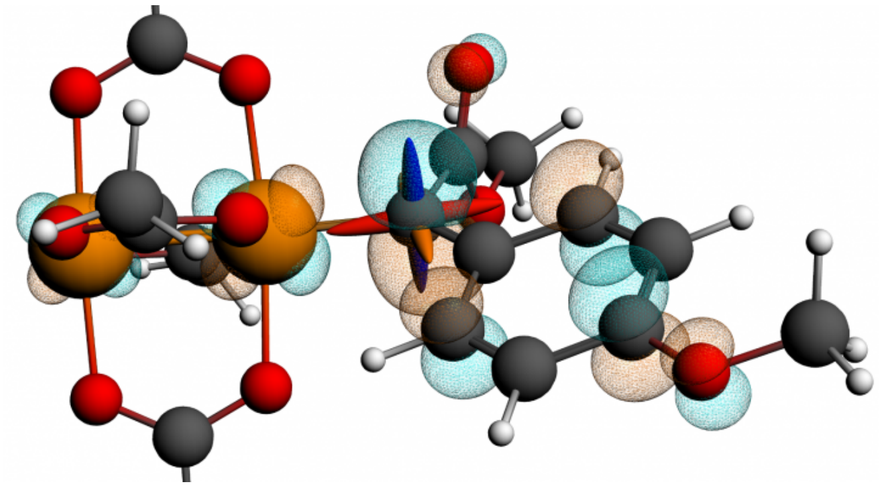
PLAMS python

Links all modules + various tools
→ workflows & screening
→ (custom) post-processing
→ rapid prototyping

ADF: Molecular DFT

Organic electronics





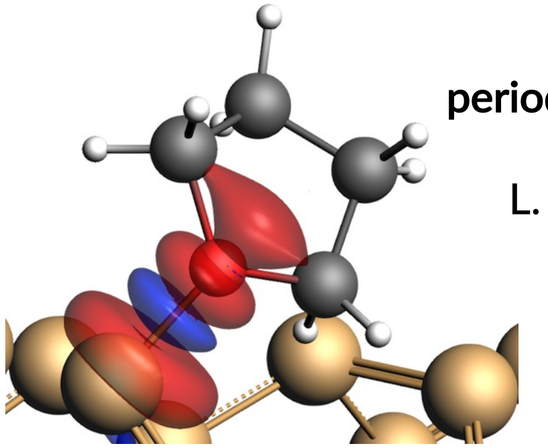
NMR calculations locate ^{13}C di-Rh carbene catalyst intermediate, Science, **342**, 351 (2013)

Strong & unique points

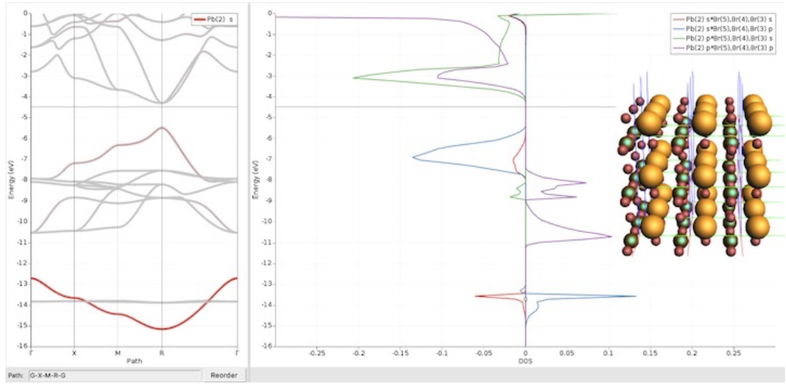
- All-electron Slaters, H-Og
- Relativity: ZORA (SR, **SOC**)
- Spectroscopy
  - EPR, NMR, IR (VCD), UVVIS, XAS
  - **Phosphorescence**
- Bonding analysis:
  - Fragment-based approach
  - ETS-NOCV, QTAIM, MO diagrams, NCI, ...
  - Transfer integrals (**charge mobility**)
- Environments
  - Subsystem DFT (FDE), **DIM/QM**, QM/MM

Periodic DFT: BAND vs Plane Waves

- Atom centered basis functions, STO or NAO
  - Compare cluster with periodic
  - No pseudopotentials, all elements
  - Core spectroscopy (core holes)
  - Easy orbital **analysis:** pDOS, COOP, EDA
  - Fast for empty (1D, 2D, porous)
  - xc: SCAN, MN15-L, HSE06, GLLB-sc, D3(BJ), DFT-1/2
  - Self-consistent NEGF
    - Gate & bias potential
    - Spin transport

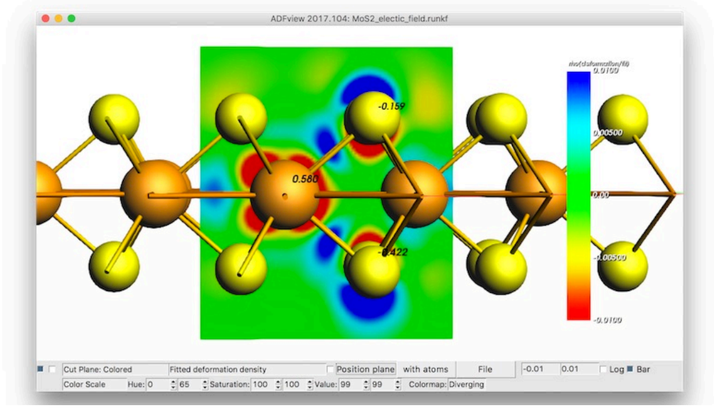


periodic energy decomposition analysis (tutorial)
L. Pecher and R. Tonner
WIREs CMS, (2018)



COOP in perovskites (tutorial)
Goesten & Hoffmann
JACS (2018)

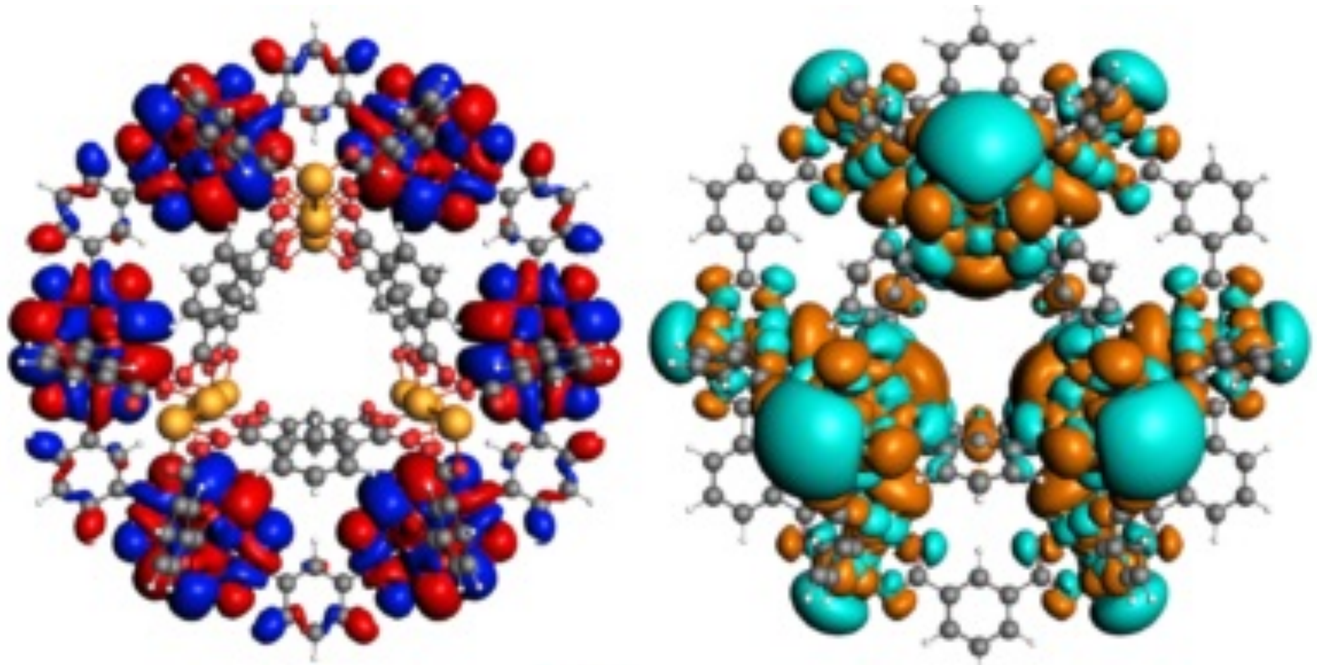
- True 2D surfaces, 1D polymers
  - Het. catalysis: polarization, COSMO, **SM12**
  - 2D electronics (homogeneous E field)
  - Nanotubes



Polarizing 2D semiconductor (tutorial)
N. Zibouche et al.
PCCP (2014)

- Integrated Graphical Interface:
  - Easy set up & analysis
  - Switch: ADF, BAND & Quantum Espresso, VASP

DFTB: ‘fast DFT’ for molecules & periodic



Approximated DFT

- Nearest neighbor & minimal basis
- Tabulated elec & rep. parameters:
  - Grimme GFN-xTB (Z = 1-86)
  - QuasiNaNo & DFTB.org

Capabilities & Features

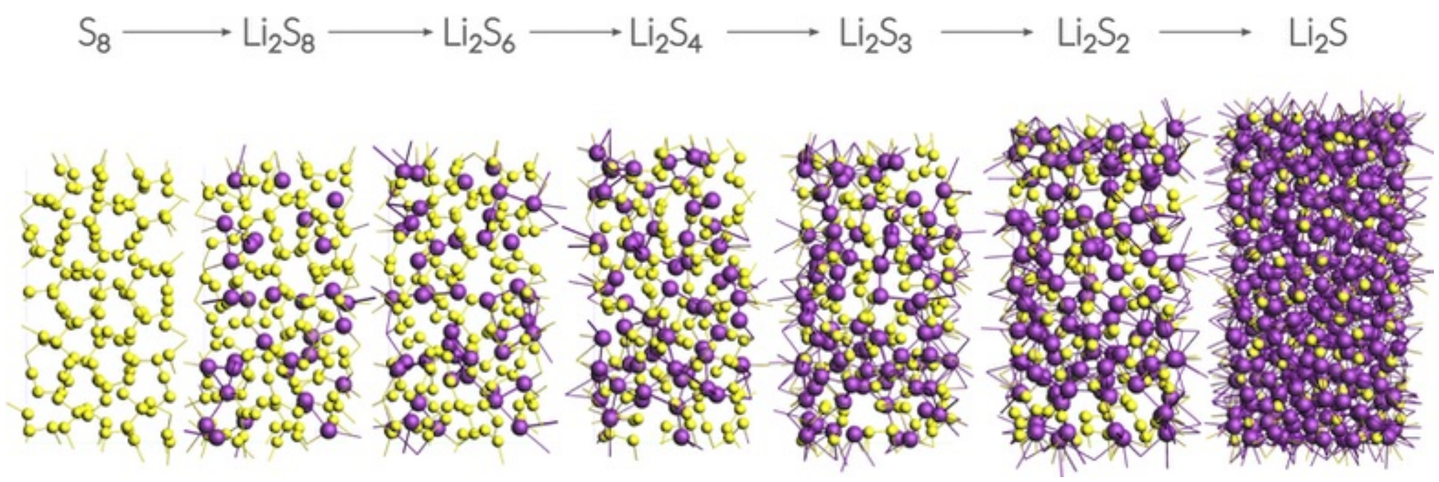
- UV/VIS (fast!)
- MOs
- (Band structures, DOS)

Through AMS

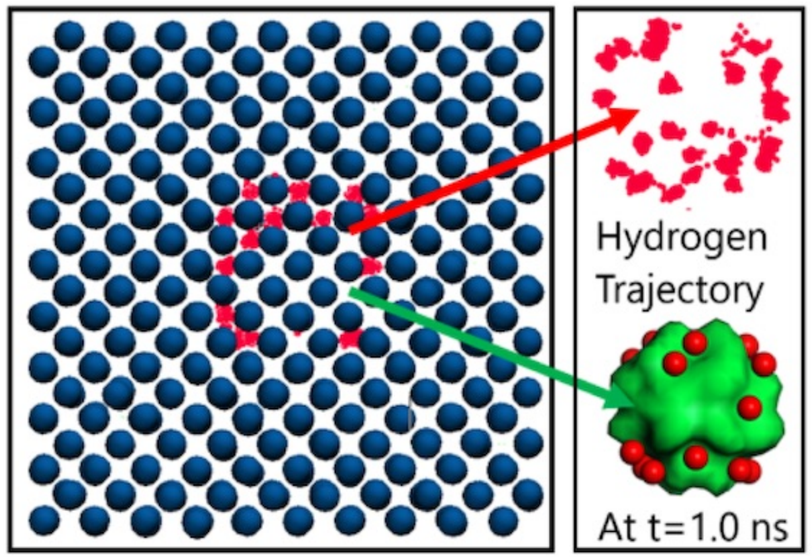
- Geometries, frequencies, phonons
- Stress tensors (optimize under p)
- Advanced MD, PES scans
- GCMC, molecule gun

Also: MOPAC library

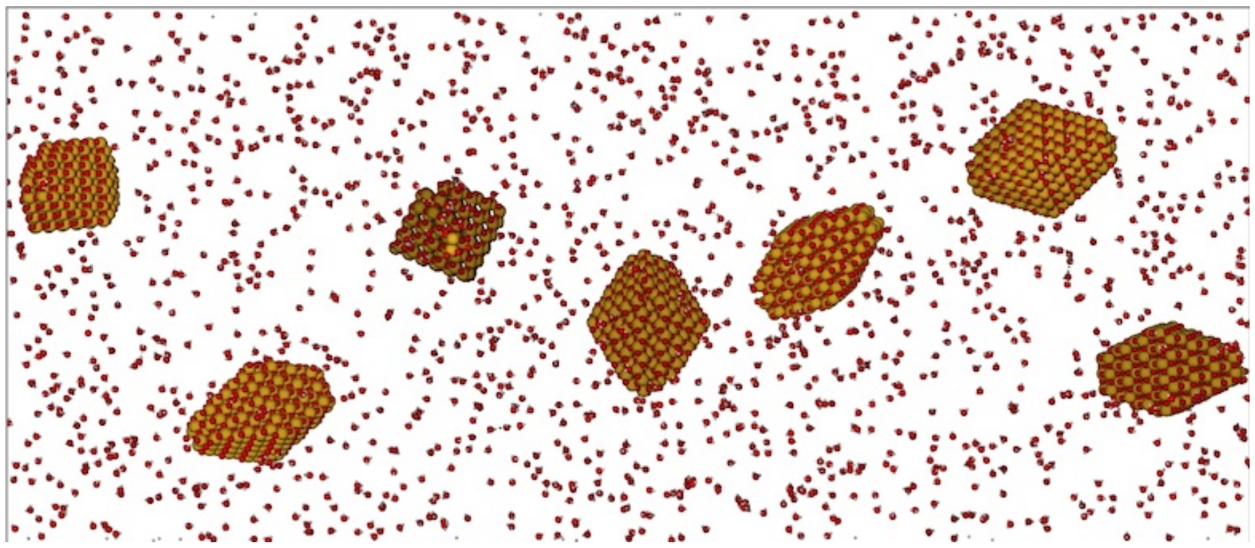
ReaxFF – reactive molecular dynamics



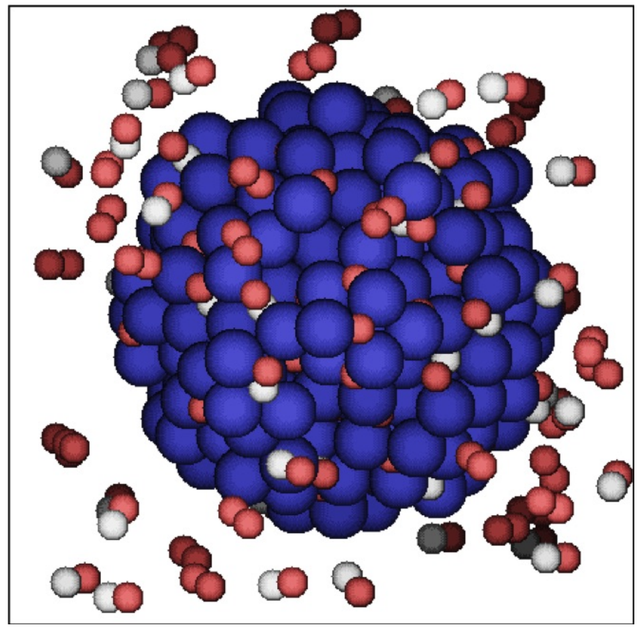
Li battery discharge: J. Electrochem. Soc. **161**, E3009 (2014); PCCP, **17**, 3383 (2015), tutorial



Hydrogen embrittlement of steels
Phys. Chem. Chem. Phys. 18 761 (2016)



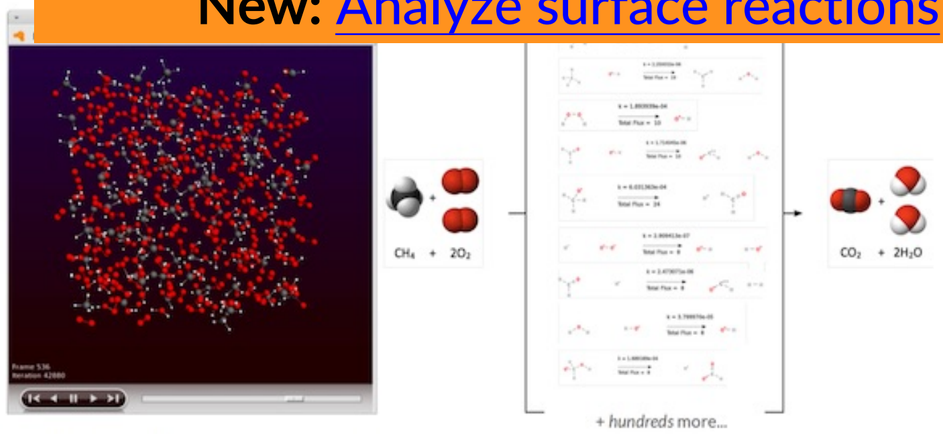
Crystallization TiO_2 nano-particles in water
Nano Lett. **14**, 1836-1842 (2014)



Pd-catalysed CO oxidation GCMC+ReaxFF
J. Chem. Phys., **139** 044109 (2013)

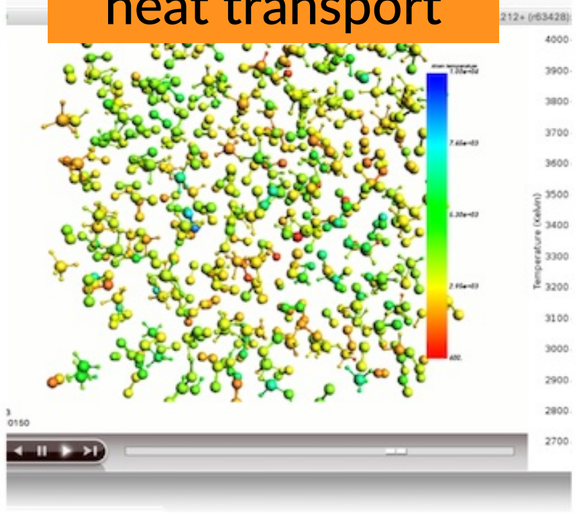
ReaxFF tools in Amsterdam Modeling Suite

ChemTraYzer: Automated rates & pathways
New: Analyze surface reactions

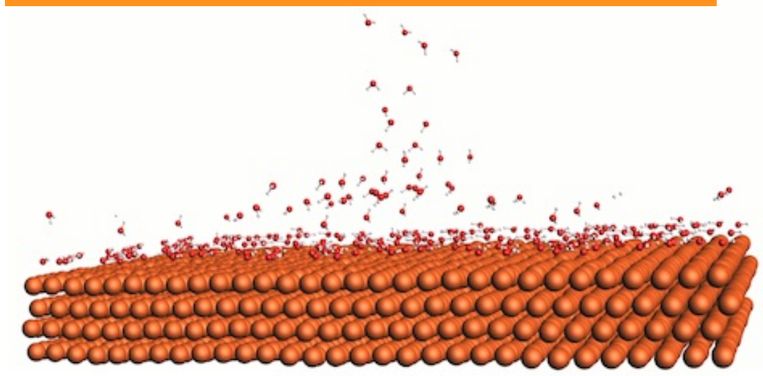


Tools += complete reaction networks
elementary reactions, rate constants, fluxes, timeline

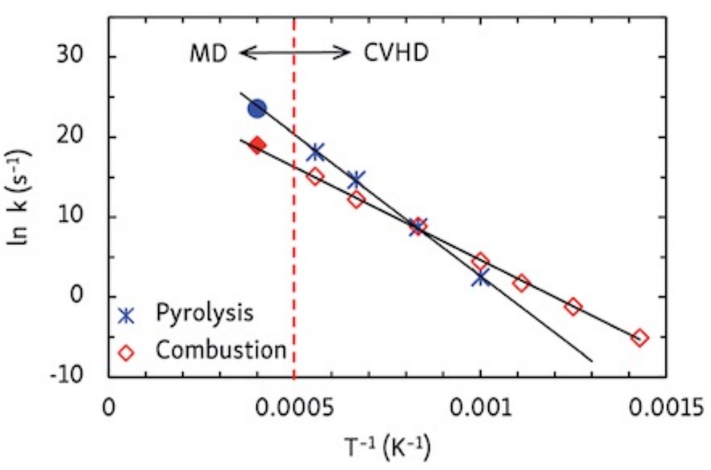
T-NEMD, local T:
heat transport

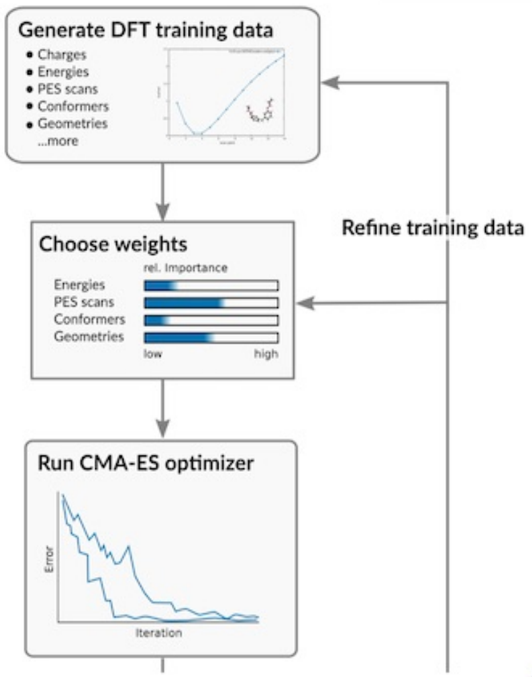


Molecule gun: depositing molecules on surfaces

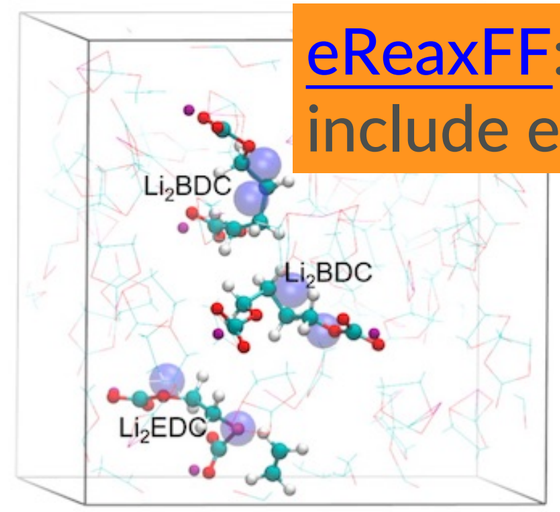


fbMC, CVHD, PRD:
speed up kinetics

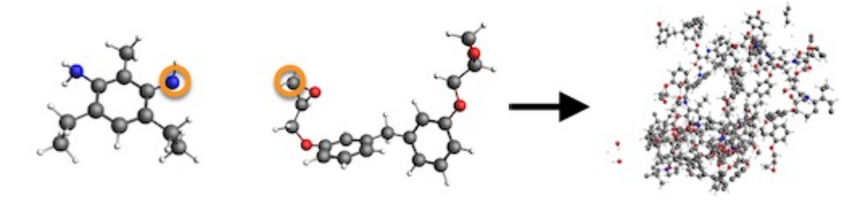




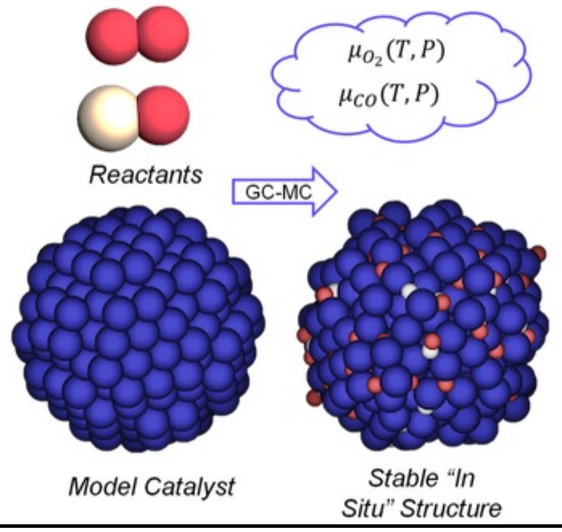
CMA-ES ReaxFF force field (re)parameterization

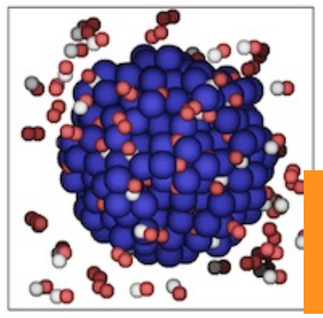


eReaxFF: include e-



bond boost
build polymers





GCMC: speed up thermo

COSMO-RS/SAC: thermodynamic properties of fluids

Quantum Chemistry & QSPR for quick property predictions

COntinuum Solvation MOdel + RS (Klamt), SAC (Sandler)
chemical potential => activity coefficients => instantaneous properties

- Solvation & excess energies, pKa
- Solubilities, LLE, VLE, boiling points
- Optimize mixtures: solubility, LLE
- Polymers: Flory-Huggins X